What is claimed is:

1. A method for determining the three-dimensional structure of a molecule of interest, which comprises

(a) obtaining x-ray diffraction data for crystals of said molecule of interest;

(b) selecting as a basis set an orthogonal set of at least one spherical harmonic spherical Bessel functions to represent the three dimensional electron density in the crystal, such that the number of degrees of freedom in the modeled electron density is reduced relative to the number of measured data;

(c) determining the maximum minimal resolution of said spherical harmonic spherical Bessel model to be used to determine the three-dimensional structure of said molecule of interest;

(d) determining a radius and position for a spherical asymmetric unit in a model crystal lattice as derived from said diffraction data for crystals;

(e) determining a computationally efficient grouping of x-ray diffraction intensities;

(f) modifying, each said at least one spherical harmonic spherical Bessel basis function within the selected basis set such that it represents an individual basis function centered at a specific position and becomes a Fourier representation of a positionally translated basis function;

(g) calculating said at least one Fourier representation of the full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function for each basis function in the basis set chosen in (b);

(h) determining at least one complex-valued coefficient of said spherical harmonic spherical Bessel series by comparing said full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function determined in (g) with said experimental x-ray diffraction data;

(i) using said at least one complex-valued coefficient of each spherical harmonic spherical Bessel function in the basis set for said spherical harmonic spherical Bessel series to iteratively update a phased Fourier representation of the 3-dimensional electron density of the crystal; and

(j) calculating Fourier summations based on a combination of said phased Fourier representation and the experimental diffraction intensities to obtain an interpretable 3-dimensional representation of the contents of the unit cell.

2. The method of claim 1 further comprising

(k) determining a modeled structure of a diffracting molecule, wherein a three-dimensional model structure of said molecule of interest by using computational graphical model fitting; and

(l) subjecting said three dimensional model structure to improvements by simulated annealing, least squares, maximum entropy, and/or Bayesian data analysis and/or molecular mechanics energy minimizations.

3. The method of claim 1 wherein said radius and position for a spherical asymmetric unit is known.

4. The method of claim 1 wherein said radius and position for a spherical asymmetric unit is not known.

5. The method of claim 4 further comprising calculation of said radius and position of said largest spherical asymmetric unit that can fit into a predetermined crystal lattice without overlap.

6. The method of claim 5 further comprising determining the numerical value of the angular increment between each trial value estimated for the phase angle of coefficient of a spherical harmonic spherical Bessel component basis function of said model of said largest spherical asymmetric unit.

7. The method of claim 5 further comprising determining the value of the spherical harmonic spherical Bessel coefficient.

8. The method of claim 1 further comprising determining the total number of m-indices to be provided in a recursive calculation.

9. The method of claim 1 further comprising determining a starting and a final value of an arbitrary exponent by which power to raise the values of calculated correlation coefficients to allow iterative improvement of the modeled electron density.

10. The method of claim 1 further comprising determining said at least one spherical Bessel function of together with ordinate values of a Bessel function argument such that the zeroes of these Bessel functions are calculated.

11. The method of claim 8 further comprising converting said diffraction m-indices to spherical coordinates and initialing said numerical values associated with said diffraction index to allow later recursive calculation of a value of each spherical harmonic Bessel basis function at said diffraction indices.

12. The method of claim 11 further comprising executing a recursive program cycle wherein unphased diffraction amplitudes are converted to a Fourier transform of a calculated model of a portion of a crystal unit cell.

13. The method of claim 1, wherein the results of said method can be further used to accurately predict the identity of ligands or to assess the relative binding affinity of said ligands to said molecule of interest.

14. The method of claim 1, wherein the process for carrying out the elements of said method for determining the three-dimensional structure of a molecule of interest, is contained in a computer, said computer being capable of receiving data and performing said method.

15. The method of claim 15, wherein said computer is coupled to a display device and there exists a means for presenting the chemical or molecular structural characteristics of said at least one molecule of interest on said display device.

16. The method of claim 1, wherein said at least one molecule of interest is selected from the group consisting of:

a) a pharmaceutical;

b) an enzyme;

c) a catalyst;

d) a polypeptide;

e) an oligopeptide;

f) a carbohydrate;

g) a nucleotide;

h) a macromolecular compound;

i) an organic moiety of an alkyl, cycloalkyl, aryl, aralkyl or alkaryl group or a substituted or heterocyclic derivative thereof;

j) an industrial compound;

k) a polymer;

l) a monomer;

m) an oligomer;

n) a polynucleotide;

o) a multimolecular aggregate; and

p) an oligopeptide.

17. The method of claim 1, wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the molecular features of said molecular object such that said representation could be used to determine desirable chemical characteristics of said at least one molecule of interest.

18. The method of claim 1, wherein the structural characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the molecular features of said molecular object such that said representation could be used to determine structural characteristics of said at least one molecule of interest that could be modified.

19. The method of claim 1, wherein said method is further utilized to predict the chemical activity of at least one molecule of interest.

20. The method of claim 1, wherein said method is further utilized to predict the biochemical activity of at least one molecule of interest.

21. The method of claim 1, wherein said method is further utilized to predict the physiological activity of at least one molecule of interest.

22. The method of claim 1 further comprising depicting a three-dimensional structure of said molecule of interest from the summation of said at least one Fourier representation.

23. The method of claim 22 further comprising generating a three-dimensional model structure of said molecule of interest from said three-dimensional structure of said molecule of interest from the summation of said at least one Fourier representation.

24. A molecule of interest as identified through the method of claim 1.

25. The molecule of interest of claim 24 wherein said molecule of interest is determined to have some chemotherapeutic activity.

26. The molecule of interest of claim 24 wherein said molecule of interest is determined to have some pharmacotherapeutic activity.

27. The molecule of interest of claim 24 wherein said molecule of interest is modified as determined by the method of claim 1 to optimize the chemotherapeutic characteristics of said molecule of interest.

28. The molecule of interest of claim 24 wherein said molecule of interest is determined to have some pharmacotherapeutic activity.

29. A molecule of interest as identified through the method of claim 1 that is determined to be effective as a therapeutic agent.

30. The molecule of interest of claim 29 wherein said molecule of interest is modified as to optimize the chemotherapeutic characteristics of said molecule of interest.

31. The molecule of interest of claim 29 wherein said molecule of interest is modified as to optimize the pharmacotherapeutic characteristics of said molecule of interest.

32. The molecule of interest of claim 30 wherein said molecule of interest is chemically modified as to optimize the chemotherapeutic characteristics of said molecule of interest.

33. The molecule of interest of claim 31 wherein said molecule of interest is chemically modified as to optimize the pharmacotherapeutic characteristics of said molecule of interest.

34. The molecule of interest of claim 30 wherein said molecule of interest is structurally modified as to optimize the chemotherapeutic characteristics of said molecule of interest.

35. The molecule of interest of claim 31 wherein said molecule of interest is structurally modified as to optimize the pharmacotherapeutic characteristics of said molecule of interest.

36. The molecule of interest of claim 29, wherein said at least one molecule of interest is selected from the group consisting of:

a) a pharmaceutical;

b) an enzyme;

c) a catalyst;

d) a polypeptide;

e) an oligopeptide;

f) a carbohydrate;

g) a nucleotide;

h) a macromolecular compound;

i) an organic moiety of an alkyl, cycloalkyl, aryl, aralkyl or alkaryl group or a substituted or heterocyclic derivative thereof;

j) an industrial compound;

k) a polymer;

l) a monomer;

m) an oligomer;

n) a polynucleotide;

o) a multimolecular aggregate; and

p) an oligopeptide.

37. The method of claim 1, wherein said x-ray diffraction data for crystals further comprises data representing the crystal space group, the crystal symmetry operators, the crystal lattice dimensions and angles, the maximum resolution of the experimental diffraction data, the experimentally measured values of the x-ray diffraction intensities, the derived values of the x-ray structure factor amplitudes, and an input value chosen for the maximum minimal resolution of the spherical harmonic, spherical Bessel (SHSB) model of said molecule of interest.

38. The molecule of interest of claim 1, wherein said molecule is Staphyloccocal nuclease.

39. The method of claim 1 further comprising inputting a numerical value for the angular increment between each trial value presumed for the phase angle of coefficient of the complex-valued individual origin-centered spherical harmonic spherical Bessel (SHSB) coefficient

40. The method of claim 1 further comprising determining an appropriate value of said angular increment automatically for each phase angle of coefficient of the complex-valued individual origin-centered spherical harmonic spherical Bessel (SHSB) coefficient.

41. The method of claim 1 further comprising:

(k) determining, from the input limiting resolution for the origin-centered spherical harmonic spherical Bessel model, the extent of the indices $_{lmn}$ of the component SHSB basis functions that are required for said molecule of interest.

(l) converting diffraction indices (hkl) to spherical coordinates,

(m) initializing some numerical values associated with each diffraction index to allow later recursive calculation of the value of each spherical harmonic spherical Bessel basis function at each hkl index; and

(n) executing a recursive program cycle.

42. The method of claim 41 further comprising:

(o) inputting the observed experimental diffraction amplitudes for each hkl index in the Fourier representation;

(p) converting a set of SHSB coefficients to at least one Fourier representation; and

(q) combining the contributions from the l, m, and n components of said at least one Fourier representation of the origin-centered, individual SHSB basis function to provide a full 3-dimensional Fourier representation of the origin-centered individual SHSB basis function of said molecule of interest.

43. The method of claim 1 further comprising writing information concerning the three dimensional Fourier representation of the model of said crystal of said molecule of interest to an electronic record keeper, the Fourier representation of each stored SHSB model such that it may be read at the beginning of the calculation for the next packet of m- values for the SHSB indices.

44. The method of claim 1, wherein the steps and calculations necessary for the determination of the depiction of said molecule of interests is capable of being recorded in an electronic medium.

45. The method of claim 1, wherein the steps and calculations necessary for the determination of the depiction of said molecule of interests is recorded in an electronic medium are stored in a secondary storage device.

46. The method of claim 1, wherein said method includes a display device such as a monitor.

47. The method of claim 43 wherein said method further provides a backup memory means to record the steps and calculations is selected from the group consisting of:

a) a floppy disk;
b) a second hard disk drive;
c) a read/write compact disc;
d) magnetic tape;
e) a Bernoulli Box;
f) a Zip disk; and
g) other means for storing electronic data

48. A method for determining the three-dimensional structure of a molecule of interest, which comprises

(a) obtaining x-ray diffraction data for crystals of said molecule of interest;

(b) choosing, as the basis set, an orthogonal set of at least one, but more often several spherical harmonic spherical Bessel functions to represent the 3-dimensional electron density in the crystal, such that the number of degrees of freedom in the modeled electron density is reduced relative to the number of measured data;

(c) determining the maximum minimal resolution of said spherical harmonic spherical Bessel model to be used to determine the three-dimensional structure of said molecule of interest;

(d) determining a radius and position for a spherical asymmetric unit in a model crystal lattice as derived from said diffraction data for crystals;

(e) determining a computationally efficient grouping of x-ray diffraction intensities;

(f) modifying, in turn, each said spherical harmonic spherical Bessel basis function within the selected basis set such that it represents an individual basis function centered at a specific position and becomes a Fourier representation of a positionally translated basis function;

(g) calculating said at least one Fourier representation of the full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function for each basis function in the basis set chosen in (b);

(h) determining the complex-valued coefficients of said spherical harmonic spherical Bessel series by comparing said full-unit cell, symmetry-expanded spherical harmonic spherical Bessel basis function determined in (g) with said experimental x-ray diffraction data;

(i) using said determined coefficients of each spherical harmonic spherical Bessel function in the basis set for said spherical harmonic spherical Bessel series to update iteratively a phased Fourier representation of the 3-dimensional electron density of the crystal; and

(j) calculating Fourier summations based on a combination of said phased Fourier representation and the experimental diffraction intensities to obtain an interpretable 3-dimensional representation of the contents of the unit cell.

wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the molecular features of said quantum object such that said representation could be used to alter to the chemical characteristics of said at least one molecule of interest.

49. The method of claim 48 wherein said spherical harmonic model to be used is the spherical Bessel mode.

50. The method of claim 48 wherein said radius and position for a spherical asymmetric unit is known.

51. The method of claim 48 wherein said radius and position for a spherical asymmetric unit is not known.

52. The method of claim 48 further comprising writing information concerning the three dimensional structure of said molecule of interest to an electronic record keeper, the Fourier representation of each stored SHSB model such that it may be read at the beginning of the calculation for the next packet of m- values for the SHSB indices.

53. The method of claim 48, wherein the steps and calculations necessary for the determination of the depiction of said molecule of interests is capable of being recorded in an electronic medium.

54. A molecule of interest as identified through the method of claim 48.

55. The molecule of interest of claim 54 wherein said molecule of interest is determined to have some chemotherapeutic activity.

56. The molecule of interest of claim 54 wherein said molecule of interest is modified as determined by the method of claim 1 to optimize the chemotherapeutic characteristics of said molecule of interest.

57. A molecule of interest as identified through the method of claim 48 that is determined to be effective as a therapeutic agent.

58. The molecule of interest of claim 57 wherein said molecule of interest is modified as to optimize the pharmacotherapeutic characteristics of said molecule of interest.

59. The molecule of interest of claim 57 wherein said molecule of interest is chemically modified as to optimize the chemotherapeutic characteristics of said molecule of interest.

60. The molecule of interest of claim 57, wherein said at least one molecule of interest is selected from the group consisting of:

a) a pharmaceutical;
b) an enzyme;
c) a catalyst;
d) a polypeptide;
e) an oligopeptide;
f) a carbohydrate;
g) a nucleotide;
h) a macromolecular compound;
i) an organic moiety of an alkyl, cycloalkyl, aryl, aralkyl or alkaryl group or a substituted or heterocyclic derivative thereof;
j) an industrial compound;
k) a polymer;

l) a monomer;

m) an oligomer;

n) a polynucleotide;

o) a multimolecular aggregate; and

p) an oligopeptide.

61. The method of claim 48, wherein the chemical characteristics of said molecule of interest are in the form of a three dimensional representation, said three dimensional representation allowing the identification of the molecular features of said quantum object such that said representation could be used to alter to the chemical characteristics of said at least one molecule of interest.

62. The method of claim 48, wherein said method is further utilized to predict the chemical activity of at least one molecule of interest.

63. A method of drug design comprising the step of using the three-dimensional structure of a molecule of interest as determined by the method of claim 1, to computationally evaluate a chemical entity for associating with the active site of a molecule of interest.

64. The method according to claim 63, wherein said chemical entity is a competitive or non-competitive inhibitor of said molecule of interest.

65. The method of drug design according to claim 63 comprising the step of using the structure coordinates of said molecule of interest to identify an intermediate in a chemical reaction between said molecule of interest and a compound which is a substrate or inhibitor of said molecule of interest.

66. The method of drug design according to claim 63, wherein said chemical entity is an inhibitor of said molecule of interest and is selected from a database.

67. The method according to claim 63, wherein said chemical entity is designed de novo.

68. The method according to claim 63, wherein said chemical entity is designed from a known inhibitor of said molecule of interest.

69. The method according to claim 63, wherein said step of employing said three-dimensional structure to design or select said chemical entity comprises the steps of:

(a). identifying molecules or molecular fragments capable of associating with molecule of interest as determined by the method of claim 1; and

(b). assembling the identified molecules or molecular fragments into a single modified molecule to provide the structure of said chemical entity.